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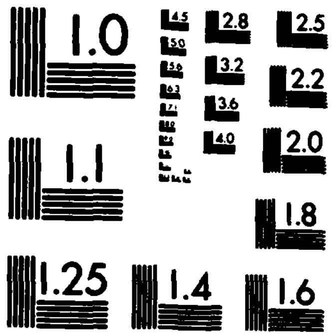

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LATTICE STATISTICS

FINAL SCIENTIFIC REPORT

GRANT AFOSR-81-0192

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FIELD	GROUP	SUB-GROUP	Lattice statistics; nearest neighbor degeneracy; dimer statistics; correlated particles; phase transitions; cooperative phenomena; recursion relationships; CONTINUED

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

The objective of this research was to develop the mathematical formalism necessary to treat a number of unsolved problems in lattice statistics. Toward that end ~~we~~ have considered the following problems: (1) The occupational degeneracy of particles of various shapes on lattice spaces of various dimensionalities and structures. (2) The nearest neighbor degeneracy for various kinds of particles on lattices spaces of various dimensionality and structures. (3) The k^{th} neighbor problem for simple particles on a one dimensional, rectangular lattice space.

Utilizing set theoretic arguments they ~~we~~ have been able to construct shift operator matrices that, in principle, permit them ~~us~~ to establish recursion relations that describe exactly the occupational degeneracy for any shape particle on a lattice space of any dimensionality and structure.

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ITEM #18, SUBJECT TERMS, CONTINUED: Fibonacci numbers; second neighbor degeneracy; third neighbor degeneracy; occupational degeneracy; lambda-bell particles; combinatorics functions; symmetric polynomials; shift operator matrices.

ITEM #19, ABSTRACT, CONTINUED: Similar techniques allow ~~us~~ the investigators to determine the composite nearest neighbor degeneracy for simple particles, dumbbells and lambda-bell particles on quasi-two dimensional rectangular lattices.

We have utilized the foregoing formalism to treat the thermodynamics [canonical and grand partition functions] for such systems.

RESEARCH OBJECTIVES AND ACCOMPLISHMENTS

The objectives of this research project are twofold:

1) To develop the mathematical formalism necessary to treat the statistics of particles distributed on lattice spaces. Of particular interest and difficulty are those situations that arise when correlation exists, either within the particle itself [as with dumbbell particles] or when the particles are allowed to interact [as with nearest neighbor interaction].

2) To utilize the aforementioned formalism in the statistical mechanical treatment of such physical and chemical phenomena as adsorption, magnetism, superconductivity and crystallization.

Accordingly we have considered a number of lattice statistics problems:

1. Occupational Degeneracy

This problem concerns a determination of the multiplicity of possible arrangements of correlated particles such as dumbbells [that occupy two linearly contiguous lattice sites], λ-bell particles [that occupy λ linearly contiguous lattice sites] as well as, for example, "L" and "T"-shaped particles, that are distributed on lattice spaces of various structures and dimensionality.

We have developed set theoretic arguments that permit the construction of shift operator matrices which, when operating on the occupational degeneracy, yield a recursion relation that describes exactly, the number of ways indistinguishable particles can be arranged on a lattice space. In principle, this technique successfully treats the occupational degeneracy problem for particles of any shape distributed on lattice spaces of any dimensionality and structure. We have utilized these results to determine the generating functions, expectation of the coverage, dispersion, normalization and continuous representation of the associated statistics for various kinds of particles distributed on rectangular and hexagonal lattice spaces.

2. The Composite k^{th} Neighbor Problem

One of the fundamental problems encountered in the mathematical treatment of lattice statistics is that of determining the complete degeneracy associated with the k^{th}-neighbor pairs created when indistinguishable particles are distributed on a lattice space. [Here k designates the order of the neighbor pair, i.e., $k = 0$ corresponds to particle occupation, $k = 1$ to nearest neighbor pairs, $k = 2$ to next nearest neighbor pairs, etc.]

Stated succinctly, the problem is as follows: Given a lattice space on which are distributed q indistinguishable particles, determine the multiplicity of those arrangements characterized by a subset of the k^{th}-neighbor pairs. [Note that the "complete" degeneracy is specified by a subset of the entire set of the various kinds of k^{th}-neighbor pairs, e.g. there are six kinds of next nearest neighbor pairs ($k = 2$), 111, 110, 101, 010, 001 and 000. For a one dimensional, rectangular lattice, there are N_k, k^{th}-neighbor pairs where

$$N_k = 2^k + 2^{[k/2]}$$

in which $[k/2]$ is the largest integer contained in $k/2$. Note here that we neglect reflective degeneracies, i.e., we count 110 but no 001.]

By a generalization of the shift operator matrix discussed here, we have been able to construct recursion relations that describe exactly the composite nearest neighbor degeneracy for simple particles and dumbbell particles distributed on quasi-two dimensional rectangular lattice spaces.

Utilizing this approach, we have also been able to construct recursion relations that describe exactly the composite nearest neighbor degeneracy for indistinguishable, simple and complex particles distributed on a 2×N lattice space. In addition we have calculated the expectation of the lattice coverage [with nearest neighbor interaction] as well as the expectation of the normalized number of nearest neighbor pairs as a function of the lattice coverage.

PUBLICATIONS

The following thirteen papers have been produced under the auspices of the Air Force under AFOSR Grant 81-0192 which was initiated 1 July 1981.

1. The Occupational Statistics for Indistinguishable Trimers on a 3×N Lattice Space (J. Math. Phys. 23, 2185 (1982)).

   This paper represents a generalization of the results for dumbbell particles for the situation arising when the indistinguishable particles occupy three linearly contiguous sites on the lattice space.

2. Exact Recursion Relation for the Occupational Degeneracy of Dumbbells on a 3×N Lattice (submitted to Journal of Combinatorial Theory).

   In this paper we develop set theoretical techniques that permit us to obtain a fourteen term recursion relationship that yields exactly the occupational degeneracy for dumbbells on a 3×N lattice space. We have also calculated the first and second moments, the generating functions, and the normalization as well as the continuous representation for the associated statistics for large values of N. One of the important aspects of this paper is that it treats the problem of a space in which some of the sites have a coordination number of four.

3. The Occupational Degeneracy for λ-bell Particles on a Saturated $\lambda \times N$ Lattice Space (Fibonacci Quarterly 24, 196 (1983)).

   A three-term, Fibonacci-like, recursion relationship is derived that describes exactly the occupational degeneracy for λ-bell particles distributed on a completely filled $\lambda \times N$ lattice space. An explicit summation representation of the saturation degeneracy is also developed and the corresponding generating functions are presented. A continuous representation for the degeneracy is given as a function of $\theta \equiv q/N$, for large values of N.

4. The Occupation Statistics for Indistinguishable Dumbbells on a 2×2×N Lattice Space (J. Math. Phys. 24, 1859 (1983)).

   This paper is concerned with the derivation of a twenty term recursion relation that describes exactly the occupation statistics for indistinguishable dumbbells distributed on a 2×2×N lattice space. On the basis of this recursion, the normalization, expectation, dispersion and continuous representation of the statistics were also developed. When the lattice space is completely filled (saturated), the recursion relationship reduces to one of four terms, permitting an exact calculation of the orientational degeneracy of a completely filled 2×2×N lattice space.

5. A Note on the Occupational Degeneracy for Dimers on a Saturated Two Dimensional Lattice Space (Discrete Applied Mathematics, 8, 101 (1984)).

Recursion relationships are developed that describe exactly the orientational degeneracy for indistinguishable dumbbells distributed on a M×N lattice space [for M = 1 through 10]. The resulting recursions yield polynomials that display a quasi-symmetry which reflects the fact that their roots exist in reciprocal pairs [or in negative reciprocal pairs]. Fundamental differences appear in the structure of these polynomials for even and odd values of M. We wish to examine these polynomials to determine whether or not they are orthogonal and if so, over what range they are orthogonal.

6. An Exact Recursion for the Composite Nearest Neighbor Degeneracy for a 2×N Lattice Space (Journal of Mathematics Physics 25, 261 (1984)).

In this paper we develop set theoretic techniques that permit us to obtain a fourteen term recursion relationship that yields exactly the composite nearest neighbor degeneracy for simple, indistinguishable particles distributed on a 2×N lattice space. We have also treated the associated generating functions as well as the expectation of the resulting statistics.

7. The Adsorption of Simple Particles on a 2×N Lattice Space (submitted to J. Vac. Sci. Tech.)

Utilizing the recursion developed under (6) above we have calculated the adsorption isotherm for simple particles distributed on a 2×N lattice. We show analytically, that the lattice coverage exhibits no discontinuity with the gas phase pressure, i.e., no phase transition can occur in such a system.

8. Mixed Nearest Neighbor Degeneracies on a 2×N Lattice Space (submitted to the Journal of Combinatorial Theory).

In this paper we determine the multiplicity of arrangements of q simple particles on a 2×N lattice that are characterized by the specification of the number of mixed nearest neighbor pairs. The associated generating functions as well as the expectation of n_{01} are also treated.

9. The Occupation Degeneracy for Dumbbells on a 3×3×N Lattice Space (submitted to Discrete Mathematics).

The 3×3×N lattice is the simplest space in which the coordination of some of the sites is that of a three dimensional lattice. Consequently, it is important to develop the occupation degeneracy of this space. We have developed a recursion that yields the multiplicity of dumbbell arrangements. Our discussion also includes a treatment of the occupational degeneracy for dumbbells on a saturated 3×3×N lattice.

10. Nearest Neighbor Statistics for Dumbbells on a 2×N Lattice Space (accepted by Journal of Mathematical Physics).

    A set theoretic argument is utilized to determine a thirty one term recursion that describes exactly the composite nearest neighbor degeneracy for indistinguishable dumbbells on a rectangular 2×N lattice. The associated generating functions and the expectation of the lattice coverage and occupied nearest neighbor pair density are also determined.

    This paper is important in that it treats the nearest neighbor degeneracy of complex particles on a two dimensional space.

11. Occupational Degeneracy for Dumbbells on a Hexagonal Lattice (accepted by Journal of Mathematical Physics).

    We develop a shift operator matrix whose determinant contains all the information necessary to determine the occupational degeneracy for dumbbells on a hexagonal lattice space. The first and second moments, the generating functions, the normalization and continuous representation (for large N) of the associated statistics are determined.

    The importance of this work is that it considers a space in which some of the sites have a coordination number of six.

12. Computer Evaluation of the Determinant of Symbolic Matrices (submitted to American Journal of Physics).

    This paper involves the computer evaluation of determinants of symbolic matrices whose elements are general polynomials of degree ten or less.

13. The Density of Occupied Nearest Neighbor Pairs on a 2×N Lattice (to be submitted to Aequationes Mathematicae).

    The density of occupied nearest neighbor pairs (as well as the lattice coverage) are determined as a function of the interaction potentials, temperature and fugacity. The importance of this work is that we were the first to show analytically that no first or second order phase transitions occur on such a space.

TECHNICAL PERSONNEL

In addition to the principal investigator the following personnel have worked on this grant. The University of Wisconsin-Milwaukee has supported some of these people as part of this matching commitment.

1. Dr. Jeff Hock — Visiting Professor

   Dr. Hock has been extremely helpful in the analytic and computational parts of our research on correlated particles [e.g. dumbbells and λ-bell particles].

2. Ms. Deborah Swarthout — Graduate Research Assistant

   Ms. Swarthout is a physics graduate student who has worked on the research pertaining to the analytic treatment of the third nearest neighbor problems.

3. Mr. Tim Yee — Graduate Research Assistant

   Mr. Yee is a graduate student in the Department of Mathematics who has worked on analytic and computer aspects of the null nearest neighbor problem.

4. Mr. Dale Walikainen — Graduate Research Assistant

   Mr. Walikainen is a physics graduate student who has performed in some calculations in problems concerned with interacting dumbbells.

5. Mr. John Maeder — Undergraduate Research Assistant

   Mr. Maeder has helped with some computer programming and calculations necessary for the project.

6. Mr. Paul Licato — Undergraduate Research Assistant

   Mr. Licato checked some of the auxiliary calculations concerning the paper on trimers.

7. Mr. Tomo Radojicic — Undergraduate Research Assistant

   Mr. Radojicic worked on computer calculations pertaining to the null nearest neighbor problem.

Mr. D. Walikainen will receive his M.S. in December 1984. His thesis advisor was the principal investigator. The title of his thesis is, "Nearest Neighbor Statistics for Interacting Dumbbells on a 2×N Lattice." The thesis has been accepted for publication by the Journal of Mathematical Physics.

COUPLING

1. Dumbbell Statistics

   (a) R. B. McQuistan, University of Wisconsin-Milwaukee

   (b) Correspondence

   (c) Discussed the use of the combinatorics function with Professor A. J. Phares, Department of Mathematics, Villanova University.

2. Nearest Neighbor Statistics

   (a) J. L. Hock, Marquette University

   (b) Discussion

   (c) Discussed some computer techniques with Professor Martin Seitz, Marquette University.

3. Recursion Polynomials

   (a) R. B. McQuistan, University of Wisconsin-Milwaukee

   (b) Discussion and collaboration

   (c) Continuing discussions on the roots of symmetric and anti-symmetric polynomials that arise in dumbbell statistics with Professor R. L. Hall, Department of Mathematics, University of Wisconsin-Milwaukee.

4. Phase Transitions

   (a) R. B. McQuistan, University of Wisconsin-Milwaukee

   (b) Seminar

   (c) Presented seminar on two dimensional phase transitions to Laboratory for Surface Studies.

5. Correlated Statistics

   (a) R. B. McQuistan, University of Wisconsin-Milwaukee

   (b) Discussion

   (c) Held discussions on nearest neighbor statistics with Dr. J. M. Charain, Visiting Professor, Marsailles, France.

6. Epitaxy and Crystal Growth

   (a) R. B. McQuistan, University of Wisconsin-Milwaukee

   (b) Discussion

   (c) Engaged in discussions on the use of lattice statistics to describe epitaxial crystal growth in two dimensions with Professor J. H. Van der Merwe, Department of Physics, University of Pretoria.

7. Dumbbell Statistics

   (a) R. B. McQuistan, University of Wisconsin-Milwaukee

   (b) Colloquium, Department of Physics, University of Wisconsin-Milwaukee

   (c) Presented Departmental Colloquium "Statistics for Dumbbells".

8. Recursion Relations, University of Wisconsin-Milwaukee

   (a) R. B. McQuistan, University of Wisconsin-Milwaukee

   (b) Correspondence

   (c) Discussed the combinatorial function technique with A. J. Phares, Villanova University.

9. Hyperspace Statistics

   (a) R. B. McQuistan, University of Wisconsin-Milwaukee

   (b) Discussion

   (c) Held discussion with Professor H. L. De Bok, Visiting Professor, Department of Mathematics (Utrecht) on the statistics of correlated particles in hyperspaces.

10. Polynomials (from recursion relations)

   (a) R. B. McQuistan, University of Wisconsin-Milwaukee

   (b) Discussion and collaboration

   (c) Held continuing discussion with Professor R. L. Hall, Department of Mathematics, University of Wisconsin-Milwaukee, concerning the roots of symmetric polynomials.

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